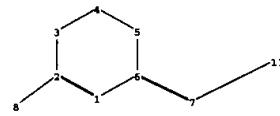
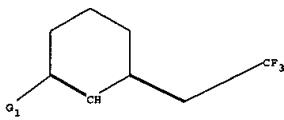


12-16-03



chain nodes :

7 8 11

ring nodes :

1 2 3 4 5 6

chain bonds :

2-8 6-7 7-11

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-2 1-6 2-3 2-8 3-4 4-5 5-6

exact bonds :

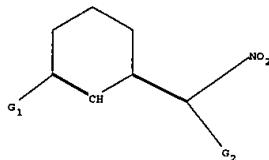
6-7 7-11

G1:C,H,O,S,N,P

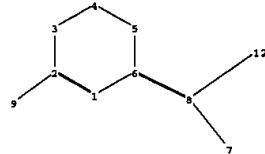
G2:C,H,O,N,p-C₆H₄,CO₂H,CN

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 11:CLASS



No answer
for the present
applied



chain nodes :
7 8 9 12

ring nodes :
1 2 3 4 5 6

chain bonds :
2-9 6-8 7-8 8-12

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6

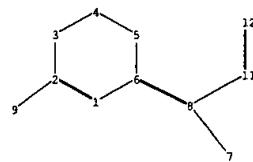
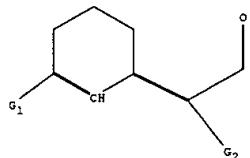
exact/norm bonds :
1-2 1-6 2-3 2-9 3-4 4-5 5-6 7-8

exact bonds :
6-8 8-12

G1:C,H,O,S,N,P

G2:C,H,O,N,p-C₆H₄,CO₂H,CN

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS



chain nodes :
7 8 9 11 12

ring nodes :
1 2 3 4 5 6

chain bonds :
2-9 6-8 7-8 8-11 11-12

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :
1-2 1-6 2-3 2-9 3-4 4-5 5-6 7-8 11-12

exact bonds :
6-8 8-11

G1:C,H,O,S,N,P

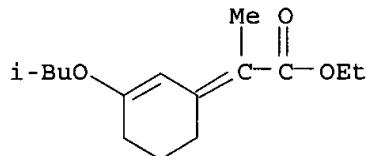
G2:C,H,O,N,p-C6H4,CO2H,CN

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS

RN 14736-74-4 REGISTRY
 CN 2-Cyclohexene-.DELTA.1,.alpha.-acetic acid, 3-isobutoxy-.alpha.-methyl-,
 ethyl ester (8CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C15 H24 O3
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier RID	RID Occurrence Count
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.2	1



Calculated Properties (CALC)

CODE	PROPERTY	VALUE	CONDITION	NOTE
HD	H donors	0		ACD (1)
HAC	H acceptors	3		ACD (1)
MW	Molecular Weight	252.35		ACD (1)
LOGP	logP	4.217+/-0.362		ACD (1)
FRB	Freely Rotatable Bonds	6		ACD (1)
LOGD	logD	4.22	pH 1	ACD (1)
LOGD	logD	4.22	pH 4	ACD (1)
LOGD	logD	4.22	pH 7	ACD (1)
LOGD	logD	4.22	pH 8	ACD (1)
LOGD	logD	4.22	pH 10	ACD (1)
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 1	ACD (1)
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 4	ACD (1)
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 7	ACD (1)
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 8	ACD (1)
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 10	ACD (1)

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2002 ACD)

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 67:2802 CA
 TI Synthesis of cyclohexane derivatives
 AU Tanaka, Tsuguo
 CS Univ. Saga, Saga, Japan
 SO Bull. Chem. Soc. Jpn. (1967), 40(1), 233-4
 CODEN: BCSJA8
 DT Journal
 LA English

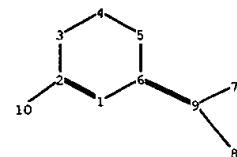
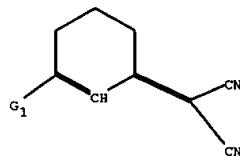
CC 24 (Alicyclic Compounds)

AB The synthesis of cyclohexane derivs. by means of the Michael condensation of 2 appropriate cyclohexane derivs. was described. Dihydroresorcinol was treated with iso-BuOH and p-toluenesulfonic acid to give an 89% yield of its isobutyl enol ether, b3 101-3.degree., which was treated with Zn and Et .alpha.-bromopropionate at 120.degree. (Reformatsky reaction) to give 50% of a product, b3 99-101.degree.. This product was hydrolyzed with HCl to give a conjugate enone, 3-(.alpha.-carbethoxyethyl)-2-cyclohexen-1-one (I), b4 123-7.degree.. The 2,4-dinitrophenylhydrazone deriv. of I was hydrogenated over 5% Pd-charcoal to give an 82.5% yield of a satd. ketone, 3-(.alpha.-carbethoxyethyl)cyclohexan-1-one (II), b3.5 111-12.degree.. The cyanohydrin of II, prep'd. by treating II with HCN, was dehydrated with SOCl₂ in a pyridine soln. at room temp. overnight. The product (44.5% yield, b3 126.5-8.5) was sepd. by vapor-phase chromatog. into 1-cyano-3-(.alpha.-carbethoxyethyl)cyclohexene and 1-cyano-5-(.alpha.- carbethoxyethyl)cyclohexene. Dimethyldihydroresorcinol was treated with HCO₂Et and Na methoxide in a C₆H₆ soln. overnight to give a 24% yield of 2,2-dimethyl-4 - hydroxymethylenecyclohexanedione 1,3 - monoethylene ketal, b4 106.0-10.5.degree..

ST CYCLOHEXENES; CYCLOHEXENONES; RESORCINOLS DIHYDRO

IT 14736-74-4P 14736-75-5P 14736-76-6P 14736-77-7P 14736-78-8P
14736-79-9P 14736-80-2P 14736-81-3P 14736-82-4P 14782-52-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prep'n. of)



chain nodes :

7 8 9 10

ring nodes :

1 2 3 4 5 6

chain bonds :

2-10 6-9 7-9 8-9

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-2 1-6 2-3 2-10 3-4 4-5 5-6

exact bonds :

6-9 7-9 8-9

G1:C,H,O

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS
10:CLASS

AN 1992:407540 CAPLUS
DN 117:7540
ED Entered STN: 11 Jul 1992
TI Reactions of trifluoromethyl ketones. VIII. Investigation of steric effect of a trifluoromethyl group through ene reaction of trifluoromethyl ketones
AU Nagai, Takabumi; Nishioka, Goro; Koyama, Mayumi; Ando, Akira; Miki, Takuichi; Kumadaki, Itsunaro
CS Fac. Pharm. Sci., Setsunan Univ., Hirakata, 573-01, Japan
SO Chemical & Pharmaceutical Bulletin (1992), 40(3), 593-8
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 22
OS CASREACT 117:7540
AB In the ene reaction of trifluoromethyl ketones, a trifluoromethyl group has been obsd. to behave as a larger substituent than commonly believed in the biomedicinal field. To est. the steric effect of a trifluoromethyl group, several trifluoromethyl ketones RCOCF_3 ($\text{R} = \text{H}, \text{Me}, \text{Bu}, \text{Ph}, \text{Me}_2\text{CHCH}_2$, cyclohexyl, EtMeCH, CF₃, thexyl) were prep'd. and their ene reaction with cyclohexene, a 1,2-disubstituted ene having the least steric requirement, examd. In this reaction, a trifluoromethyl group was found to behave as if it were a much larger substituent than a Ph or iso-Bu group and as large as a sec-Bu group.
ST steric effect trifluoromethyl group ene reaction; ketone trifluoromethyl ene reaction; stereochem ene reaction trifluoromethyl ketone; regiochem ene reaction trifluoromethyl ketone
IT Steric effect
(of trifluoromethyl group on ene reaction of trifluoromethyl ketones)
IT Trifluoromethyl group
(steric effect of, on ene reactions of trifluoromethyl ketones)
IT Addition reaction
(ene, of trifluoromethyl ketones, steric effect of trifluoromethyl group on)
IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(trifluoromethyl, ene reaction of, steric effect of trifluoromethyl group on)
IT 76-05-1, Trifluoroacetic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of)
IT 108-85-0, Cyclohexyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with iso-Bu trifluoromethyl ketone)
IT 78-77-3, Isobutyl-bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with trifluoroacetic acid)
IT 1521-51-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with trifluoroacetophenone)
IT 75-90-1, Trifluoroacetaldehyde 360-34-9 421-50-1 434-45-7,
.alpha.,.alpha.,.alpha.-Trifluoroacetophenone 684-16-2,
Hexafluoroacetone
RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, steric effect of the trifluoromethyl group in)
IT 433-27-2, Trifluoroacetaldehyde ethyl hemiacetal
RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, with dimethylbutenes)
IT 563-79-1, 2,3-Dimethyl-2-butene
RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, with trifluoroacetaldehyde)
IT 110-83-8, Cyclohexene, reactions 13389-42-9
RL: RCT (Reactant); RACT (Reactant or reagent)

(ene reaction of, with trifluoromethyl ketones)

IT 116356-54-8P 122129-36-6P 122129-38-8P 141779-27-3P 141779-28-4P
 141779-29-5P 141779-30-8P 141779-31-9P 141779-32-0P
 141779-33-1P 141779-34-2P 141779-35-3P 141779-36-4P
 141779-37-5P 141779-38-6P 141779-39-7P
 141779-42-2P 141779-43-3P 141779-44-4P 141846-75-5P 141846-76-6P
 141846-77-7P 141899-03-8P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and spectra of)

IT 114420-54-1P 122129-28-6P 122129-29-7P 122129-30-0P 122129-31-1P
 125458-29-9P 134166-51-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

IT 134166-52-2P 134166-53-3P 134166-54-4P 134166-55-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn., spectra and dehydration of)

IT 6302-04-1P, Cyclohexyl trifluoromethyl ketone 75703-02-5P, Isobutyl trifluoromethyl ketone 134166-49-7P, sec-Butyl trifluoromethyl ketone 134166-50-0P, Thexyl trifluoromethyl ketone
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn., spectra and ene reaction of, steric effect of the trifluoromethyl group in)

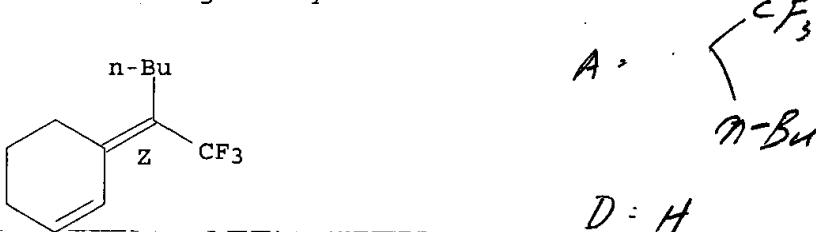
IT 141779-40-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn., spectra and hydrogenation of)

IT 141779-41-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn., spectra and oxidn. of)

IT 141779-32-0P 141779-34-2P 141779-35-3P
 141779-37-5P 141779-38-6P 141779-39-7P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and spectra of)

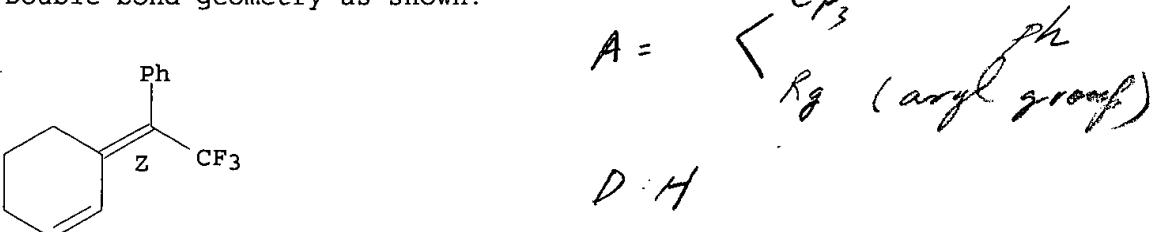
RN 141779-32-0 CAPLUS
 CN Cyclohexene, 3-[1-(trifluoromethyl)pentylidene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 141779-34-2 CAPLUS
 CN Benzene, [1-(2-cyclohexen-1-ylidene)-2,2,2-trifluoroethyl]-, (Z)- (9CI) (CA INDEX NAME)

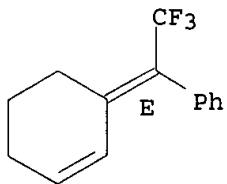
Double bond geometry as shown.



RN 141779-35-3 CAPLUS
 CN Benzene, [1-(2-cyclohexen-1-ylidene)-2,2,2-trifluoroethyl]-, (E)- (9CI)

(CA INDEX NAME)

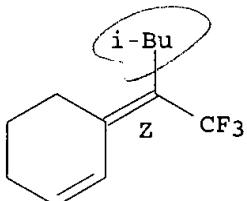
Double bond geometry as shown.



RN 141779-37-5 CAPLUS

CN Cyclohexene, 3-[3-methyl-1-(trifluoromethyl)butylidene]-, (Z)- (9CI) (CA INDEX NAME)

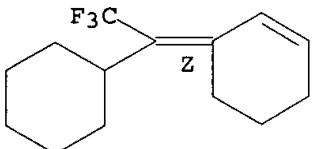
Double bond geometry as shown.



RN 141779-38-6 CAPLUS

CN Cyclohexene, 3-(1-cyclohexyl-2,2,2-trifluoroethylidene)-, (Z)- (9CI) (CA INDEX NAME)

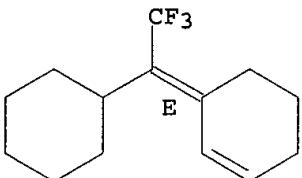
Double bond geometry as shown.



RN 141779-39-7 CAPLUS

CN Cyclohexene, 3-(1-cyclohexyl-2,2,2-trifluoroethylidene)-, (E)- (9CI) (CA INDEX NAME)

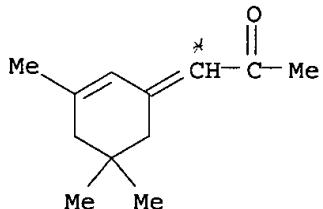
Double bond geometry as shown.



RN 3211-80-1 REGISTRY
 CN 2-Propanone, 1-(3,5,5-trimethyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX
 NAME)
 OTHER CA INDEX NAMES:
 CN 2-Propanone, (3,5,5-trimethyl-2-cyclohexen-1-ylidene)- (7CI, 8CI)
 FS 3D CONCORD
 DR 178117-22-1
 MF C12 H18 O
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMLIST, TOXCENTER
 (*File contains numerically searchable property data)
 Other Sources: EINECS**
 (**Enter CHEMLIST File for up-to-date regulatory information)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.2	1



$R_1 : H$

$R_{m,n,g,r} : H$

$R_1 : CH_3$

$D : CH_3$

$R_O \neq R_P : CH_3$

Calculated Properties (CALC)

CODE	PROPERTY	VALUE	CONDITION	NOTE
HD	H donors	0		ACD (1)
HAC	H acceptors	1		ACD (1)
MW	Molecular Weight	178.27		ACD (1)
LOGP	logP	3.334 +/- 0.241		ACD (1)
FRB	Freely Rotatable Bonds	1		ACD (1)
LOGD	logD	3.33	pH 1	ACD (1)
LOGD	logD	3.33	pH 4	ACD (1)
LOGD	logD	3.33	pH 7	ACD (1)
LOGD	logD	3.33	pH 8	ACD (1)
LOGD	logD	3.33	pH 10	ACD (1)
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 1	ACD (1)
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 4	ACD (1)
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 7	ACD (1)
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 8	ACD (1)
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 10	ACD (1)

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2002 ACD)

2 REFERENCES IN FILE CA (1967 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

AN 129:44683 CA
TI Evaluation of organic pollutants in a contaminated area
AU Rotatori, Mauro; Bertoni, Giuliano; Ferragina, Carla; Maio, Giovanni;
Tappa, Remo
CS Istituto sull'Inquinamento Atmosferico, Montelibretti, C.N.R., Rome, Italy
SO Acqua Aria (1998), (3), 109-117
CODEN: AQARDW; ISSN: 0391-5557
PB Arti Poligrafiche Europee Srl
DT Journal
LA Italian
CC 60-6 (Waste Treatment and Disposal)
Section cross-reference(s): 19, 80
AB A sampling-anal. strategy for contaminated soils which permits to collect a large amt. of quant. and qual. data in a reasonably short time is proposed. Various anal. techniques: thermal desorption-gas chromatog. anal. (TF-GC), solvent extn. followed by gas chromatog./mass-spectrometric anal. (GC-MS), thermogravimetry with DTA (TG-DTA) and powder diffractometry (XRPD) were used and compared in order to characterize samples of soils. Results of a study performed in an industrial area contaminated by unknown org. compds. were obtained. About 70 org. pollutants were identified. The vertical distribution profile of org. pollutants is discussed.
ST org pollutant contaminated soil analysis
IT Soils
 (contaminated; org. pollutant detn. in contaminated soils)
IT Sampling
 (org. pollutant detn. in contaminated soils)
IT Organic compounds, analysis
RL: ANT (Analyte); POL (Pollutant); ANST (Analytical study); OCCU (Occurrence)
 (org. pollutant detn. in contaminated soils)
IT 50-32-8, Benzo[alpyrene, analysis 78-59-1 84-66-2,
1,2-Benzenedicarboxylic acid, diethyl ester 84-69-5,
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester 85-01-8,
Phenanthrene, analysis 88-69-7 91-20-3, Naphthalene, analysis 95-63-6, 1,2,4-Trimethylbenzene 98-82-8, 1-Methylethylbenzene 99-87-6,
1-Methyl-4-(1-methylethyl)-benzene 100-51-6, Benzenemethanol, analysis 100-52-7, Benzaldehyde, analysis 100-53-8, Benzeneméthanethiol 103-29-7 103-65-1, Propylbenzene 108-10-1, 4-Methyl-2-pentanone 111-82-0,
Dodecanoic acid, methyl ester 111-84-2, Nonane 112-40-3, Dodecane 117-81-7, 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester 120-61-6
, 1,4-Benzenedicarboxylic acid, dimethyl ester 122-57-6 123-42-2
124-18-5, Decane 129-00-0, Pyrene, analysis 141-93-5,
1,3-Diethylbenzene 150-78-7, 1,4-Dimethoxybenzene 198-55-0, Perylene 206-44-0, Fluoranthene 207-08-9, Benzo[k]fluoranthene 218-01-9,
Chrysene 301-02-0 496-11-7, 2,3-Dihydro-1H-indene 504-20-1
514-94-3, 1,5,5,6-Tetramethyl-1,3-cyclohexadiene 514-96-5,
1,2,6,6-Tetramethyl-1,3-cyclohexadiene 526-73-8, 1,2,3-Trimethylbenzene 535-77-3, 1-Methyl-3-(1-methylethyl)benzene 538-58-9,
1,5-Diphenyl-1,4-pentadien-3-one 546-49-6, 3,3,6-Trimethyl-1,5-heptadien-4-one 586-62-9 604-53-5, 1,1'-Binaphthalene 611-14-3,
1-Ethyl-2-methylbenzene 612-78-2, 2,2'-Binaphthalene 620-14-4,
1-Ethyl-3-methylbenzene 622-96-8, 1-Ethyl-4-methylbenzene 629-50-5,
Tridecane 629-59-4, Tetradecane 1074-17-5, 1-Methyl-2-propylbenzene 1074-43-7, 1-Methyl-3-propylbenzene 1090-13-7, 5,12-Naphthacenedione 1120-21-4, Undecane 1193-18-6, 3-Methyl-2-cyclohexen-1-one 1515-95-3,
1-Ethyl-4-methoxy-benzene 2464-33-7 2819-61-6 3211-80-1 3212-51-9
3431-87-6 3561-67-9 3637-01-2, 1-(3,4-Dimethylphenyl)-ethanone 4325-74-0, 1,2'-Binaphthalene 17851-53-5, 1,2-Benzenedicarboxylic acid, butyl-2-methylpropyl ester 62968-85-8 66378-50-5, 2-Acetyl-2-carene 72535-88-7 74381-40-1, Propanoic acid, 2-methyl-,1(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester 77822-60-7 197390-29-7 208179-76-4
RL: ANT (Analyte); POL (Pollutant); ANST (Analytical study); OCCU (Occurrence)

(org. pollutant detn. in contaminated soils)

REFERENCE 2

AN 125:41250 CA
TI Analysis of extractable organic compounds in water by gas chromatography mass spectrometry: applications to surface water
AU Deroux, J. M.; Gonzalez, C.; Le Cloirec, P.; Kovacsik, G.
CS Lab. Genie Environ. Ind., Ecole Mines Ales, Fr.
SO Talanta (1996), 43(3), 365-380
CODEN: TLNTA2; ISSN: 0039-9140
DT Journal
LA English
CC 61-3 (Water)
Section cross-reference(s): 80
AB Over a period of 1 yr, the surface water of a canal network (Languedoc-Roussillon area, France) was analyzed in order to identify org. compds. and to monitor its quality. Pollutants were extd. from 19 L of raw water using methylene chloride in a continuous countercurrent liq.-liq. extractor with a pulsed column. The extn. was performed at a pH above 11 and again at a pH below 2 according to U.S. Environmental Protection Agency method 625. The ext. was analyzed by gas chromatog./mass spectrometry, using two ionization techniques, namely electron ionization and chem. ionization. Mass spectra obtained by electron ionization were compared with those in a database (NIST). Some natural compds. and micropollutants were identified. Their structures were confirmed by chem. ionization (methane). One hundred and ten substances, making up the broad spectrum of extractable compds. in the surface water studied, were found by this method at a nanogram per L concn. level. Among them, 13 are priority pollutants. These specific pollutants were qualified.
ST extractable org detn surface water GCMS
IT Water pollution
 (anal. of extractable org. compds. in water by gas chromatog. mass spectrometry: applications to surface water)
IT Chlorides, analysis
 RL: ANT (Analyte); ANST (Analytical study)
 (anal. of extractable org. compds. in water by gas chromatog. mass spectrometry: applications to surface water)
IT Pesticides
 (detn. of extractable org. compds. in surface water by gas chromatog. mass spectrometry)
IT Alcohols, analysis
Aldehydes, analysis
Amines, analysis
Aromatic hydrocarbons, analysis
Ketones, analysis
Phenols, analysis
 RL: ANT (Analyte); ANST (Analytical study)
 (detn. of extractable org. compds. in surface water by gas chromatog. mass spectrometry)
IT Organic compounds, analysis
 RL: ANT (Analyte); ANST (Analytical study)
 (sulfur-contg., anal. of extractable org. compds. in water by gas chromatog. mass spectrometry: applications to surface water)
IT 74-82-8, Methane, analysis 75-09-2, analysis 7440-61-1, Uranium, analysis 7704-34-9D, Sulfur, org. compds.
 RL: ANT (Analyte); ANST (Analytical study)
 (anal. of extractable org. compds. in water by gas chromatog. mass spectrometry: applications to surface water)
IT 62-53-3, Benzenamine, analysis
 RL: ANT (Analyte); ANST (Analytical study)
 (derivs; detn. of extractable org. compds. in surface water by gas chromatog. mass spectrometry)

IT 7732-18-5, Water, analysis
RL: AMX (Analytical matrix); ANST (Analytical study)
(detn. of extractable org. compds. in surface water by gas chromatog.
mass spectrometry)

IT 51-28-5, analysis 58-08-2, analysis 58-89-9 65-85-0, Benzoic acid,
analysis 78-40-0 80-46-6 83-32-9 83-33-0 86-73-7, 9H-Fluorene
87-28-5 87-41-2, 1(3H)-Isobenzofuranone 87-61-6 87-65-0 88-06-2
88-72-2 88-75-5 88-85-7 89-64-5 91-56-5, 1H-Indole-2,3-dione
91-64-5, 2H-1-Benzopyran-2-one 92-48-8, 6-Methyl-2H-1-benzopyran-2-one
95-65-8 95-76-1 98-54-4 98-73-7, p-tert-Butylbenzoic acid 98-95-3,
analysis 99-30-9 99-52-5 99-54-7 99-96-7, analysis 99-99-0
100-00-5 100-18-5 100-46-9, Benzenemethanamine, analysis 101-84-8
103-69-5 115-96-8 120-12-7, Anthracene, analysis 121-14-2 122-34-9
122-95-2 127-51-5 130-15-4, 1,4-Naphthalenedione 132-64-9,
Dibenzofuran 137-17-7 140-67-0 150-78-7 206-44-0, Fluoranthene
298-00-0 487-48-9 496-15-1 497-56-3, 2-Methyl-3,5-dinitrophenol
523-80-8 529-16-8, 2,3-Dimethyl-bicyclo[2.2.1]hept-2-ene 583-60-8
606-20-2 609-89-2 611-06-3 611-92-7 618-45-1,
3-(1-Methylethyl)phenol 619-08-9 620-02-0,
5-Methyl-2-furancarboxaldehyde 620-83-7, 1-Methyl-4-
(phenylmethyl)benzene 634-93-5 696-23-1 700-38-9 759-22-8,
N,N'-Bis(1-methylethyl)acetamide 816-16-0 825-41-2 873-94-9
931-54-4 1125-21-9 1195-79-5, 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-
one 1635-02-5 1689-64-1, 9H-Fluoren-9-ol 1817-47-6,
1-(1-Methylethyl)-4-nitrobenzene 1912-24-9 1984-65-2 2189-60-8
2605-67-6, (Triphenylphosphoranylidene) methyl acetate 2683-43-4
3211-80-1 3302-10-1 3552-33-8 5590-14-7,
2-Phenyl-trans-cyclopropanecarbonitrile 5715-23-1 5915-41-3
6333-37-5 6341-97-5 6781-42-6 7051-39-0 7789-92-6 10298-80-3
13524-76-0, 3,3-Dimethyl-2(3H)-benzofuranone 13757-91-0 15176-21-3
15356-74-8 15972-60-8 17699-14-8, .alpha.-Cubebene 20547-99-3
20895-41-4, 6-Methyl-3(2H)-benzofuranone 21303-80-0,
Dihydro-5-methyl-5-phenyl-2(3H)-furanone 22841-82-3 26271-75-0,
4-Amino-3,5-dichlorophenol 26545-51-7 51218-45-2 53543-47-8
54120-64-8 160498-63-5, 2,3-Dihydro-2,3-dimethyl-7-benzofuranol
RL: ANT (Analyte); ANST (Analytical study)
(detn. of extractable org. compds. in surface water by gas chromatog.
mass spectrometry)

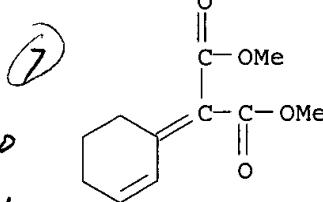
RN 122471-20-9 REGISTRY
 CN Propanedioic acid, 2-cyclohexen-1-ylidene-, dimethyl ester (9CI) (CA
 INDEX NAME)
 FS 3D CONCORD
 MF C11 H14 O4
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, GMELIN*
 (*File contains numerically searchable property data)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier RID	RID Occurrence Count
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.2	1

cl 1.

4.

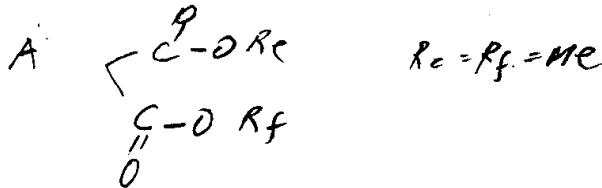


D \rightarrow H

$\alpha_1, \alpha, \alpha, \alpha, p, \beta, r = H$

41

(2)(5)



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	33.9	pH 1	(1) ACD
Bioconc. Factor (BCF)	33.9	pH 4	(1) ACD
Bioconc. Factor (BCF)	33.9	pH 7	(1) ACD
Bioconc. Factor (BCF)	33.9	pH 8	(1) ACD
Bioconc. Factor (BCF)	33.9	pH 10	(1) ACD
Boiling Point (BP)	258.1 +/- 13.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	49.57 +/- 3.0 kJ/mol		(1) ACD
Flash Point (FP)	119.6 +/- 32.8 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	4		(1) ACD
H acceptors (HAC)	4		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	433	pH 1	(1) ACD
Koc (KOC)	433	pH 4	(1) ACD
Koc (KOC)	433	pH 7	(1) ACD
Koc (KOC)	433	pH 8	(1) ACD
Koc (KOC)	433	pH 10	(1) ACD
logD (LOGD)	2.32	pH 1	(1) ACD
logD (LOGD)	2.32	pH 4	(1) ACD
logD (LOGD)	2.32	pH 7	(1) ACD
logD (LOGD)	2.32	pH 8	(1) ACD
logD (LOGD)	2.32	pH 10	(1) ACD
logP (LOGP)	2.316 +/- 0.350		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD

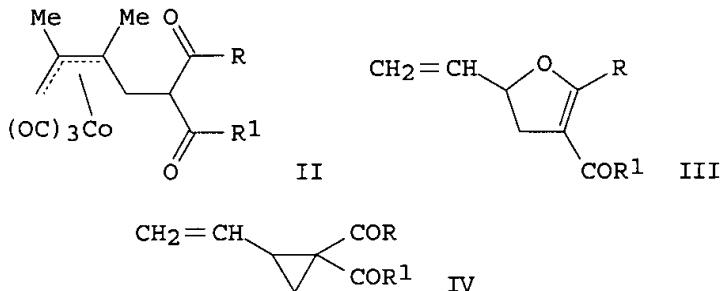
Molecular Weight (MW)	210.23		(1) ACD
Vapor Pressure (VP)	0.0139633 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 111:154088 CA
TI Deprotonation of the adducts of .beta.-dicarbonyl anions and
[(.eta.4-diene)Co(CO)₃]BF₄
AU Barinelli, Lucio S.; Li, Zhong; Nicholas, Kenneth M.
CS Dep. Chem. Biochem., Univ. Oklahoma, Norman, OK, 73019, USA
SO Organometallics (1989), 8(10), 2474-6
CODEN: ORGND7; ISSN: 0276-7333
DT Journal
LA English
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 24, 27
GI



AB The adducts of stabilized enolates and [(η .4-1,3-butadiene)Co(CO)₃]BF₄ (I) and [(η .4-1,3-cyclohexadiene)Co(CO)₃]BF₄ undergo deprotonation and subsequent reactions to form either hydrofuran, cyclopropanes, or α , β , γ , δ -diunsatd. dicarbonyl derivs. depending upon the reacting complex and the β -dicarbonyl component. All of the obsd. reactions are strongly promoted by HMPA. Thus, treatment of the adducts II (R = Me, R₁ = Ph, OMe; R = R₁ = OMe), formed from reaction of I and RCOCH₂C(ONA)R₁, with LiN(CHMe₂)₂ in the presence of HMPA give dihydrofurans III (R = Me, R₁ = Ph, OMe) or cyclopropane IV (R = R₁ = OMe).

ST enolate dienecobalt alkylation; deprotonation dienecobalt enolate adduct cyclization; HMPA deprotonation catalyst dienecobalt enolate adduct; hydride shift dienecobalt enolate adduct; dihydrofuran vinyl acyl; cyclopropane vinyl diacyl

IT Ring closure and formation
(in deprotonation of adducts of stabilized enolates with (diene)cobalt tricarbonyl cations)

IT Hydride shift
(1,4-, in deprotonation reactions of adducts of .beta.-dicarbonyl anions with (diene)cobalt tricarbonyl cations)

IT Protonation catalysts
(deprotonation, HMPA, for adducts of .beta.-dicarbonyl anions and
(diene)cobalt tricarbonyl cations)

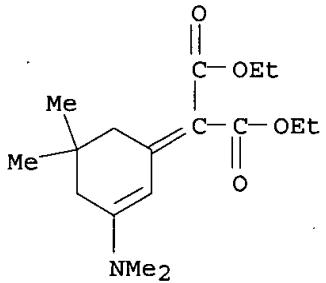
- IT Protonation and Proton transfer reaction
(deprotonation, of adducts of .beta.-dicarbonyl anions and
(diene)cobalt tricarbonyl cations)
- IT 623-58-5, Sodium acetoacetate 17664-05-0, Sodium benzoylacetonate
18424-76-5, Sodium dimethyl malonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of enolate adducts of (diene)cobalt tricarbonyl
cations)
- IT 680-31-9, HMPA, uses and miscellaneous
RL: CAT (Catalyst use); USES (Uses)
(catalyst, in deprotonation of enolate adducts of (diene)cobalt
tricarbonyl cation)
- IT 33009-59-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cleavage of, (dimethylbutadiene)cobalt tricarbonyl cation from)
- IT 1333-74-0 12184-88-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydride shift, 1,4-, in deprotonation reactions of adducts of
.beta.-dicarbonyl anions with (diene)cobalt tricarbonyl cations)
- IT 122471-24-3P 122471-25-4P 122471-27-6P 122471-28-7P 122471-29-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and deprotonation of)
- IT 122471-22-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and C-alkylation of, with stabilized enolates)
- IT 17447-60-8P 34939-28-1P 88326-56-1P 113949-31-8P 115740-69-7P
122471-14-1P 122471-15-2P 122471-16-3P 122471-17-4P 122471-18-5P
122471-19-6P 122471-20-9P 122471-26-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 122471-23-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn., hydrolysis, and deprotonation of)
- IT 12408-02-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(protonation and Proton transfer reaction, deprotonation, of adducts of
.beta.-dicarbonyl anions and (diene)cobalt tricarbonyl cations)
- IT 90502-48-0 113949-35-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(C-alkylation of, with stabilized enolates)

RN 31039-90-4 REGISTRY
 CN 2-Cyclohexene-.DELTA.1,.alpha.-malonic acid, 3-(dimethylamino)-5,5-dimethyl-, diethyl ester (8CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C17 H27 N O4
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.2	1

cl /



D = NR_aR_b R_a=R_b=Me

R_a, R_b = CH₃

A =

R_c = R_f = Et

Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1.57	pH 4	(1) ACD
Bioconc. Factor (BCF)	435	pH 7	(1) ACD
Bioconc. Factor (BCF)	774	pH 8	(1) ACD
Bioconc. Factor (BCF)	846	pH 10	(1) ACD
Boiling Point (BP)	359.3 +/- 42.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	60.48 +/- 3.0 kJ/mol		(1) ACD
Flash Point (FP)	171.1 +/- 50.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3.45	pH 1	(1) ACD
Koc (KOC)	8.01	pH 4	(1) ACD
Koc (KOC)	2226	pH 7	(1) ACD
Koc (KOC)	3961	pH 8	(1) ACD
Koc (KOC)	4332	pH 10	(1) ACD
logD (LOGD)	1.06	pH 1	(1) ACD
logD (LOGD)	1.42	pH 4	(1) ACD
logD (LOGD)	3.87	pH 7	(1) ACD
logD (LOGD)	4.12	pH 8	(1) ACD
logD (LOGD)	4.15	pH 10	(1) ACD
logP (LOGP)	4.156 +/- 0.387		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD

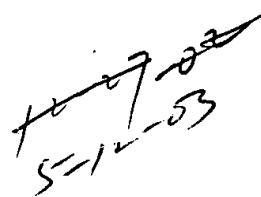
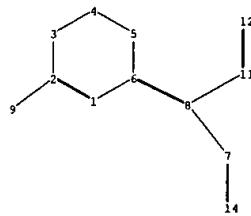
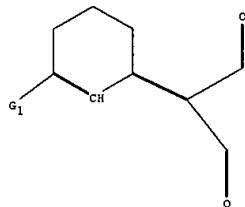
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	309.40		(1) ACD
pKa (PKA)	6.98+-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	2.41E-05 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 74:12468 CA
 TI Hindered internal rotation in some enamines
 AU Dahlqvist, Kjell I.; Forssen, Sture
 CS Chem. Cent., Lund Inst. Technol., Lund, Swed.
 SO Acta Chemica Scandinavica (1947-1973) (1970), 24(6), 2075-83
 CODEN: ACSAA4; ISSN: 0001-5393
 DT Journal
 LA English
 CC 22 (Physical Organic Chemistry)
 GI For diagram(s), see printed CA Issue.
 AB The hindered internal rotation of the N,N-dimethyl group in I, II, and III was studied by NMR at 60 and 100 MHz. The interconversion rate was evaluated by iterative fitting of the theoretical spectra to the exptl. spectra using digital computer. The free energy of activation (.DELTA.F.++) for the hindered internal rotation of NMe in the compds. studied depends on the exocyclic substituent in the order :C(COOEt)2 <:O <:C(CN)2. The entropies of activation had large pos. values.
 ST cyclohexene enamines hindered internal rotation; enamines cyclohexene hindered internal rotation; hindered internal rotation cyclohexene enamines
 IT Amines, properties
 RL: PRP (Properties)
 (enamines, potential barrier to rotation of)
 IT Entropy
 Free energy
 (of activation, of rotation of enamines)
 IT Potential barriers
 (rotational, of enamines)
 IT 31039-88-0 31039-89-1 31039-90-4
 RL: PRP (Properties)
 (potential barrier to rotation of)
 IT 31039-91-5P 31039-92-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)



chain nodes :
7 8 9 11 12 14

ring nodes :
1 2 3 4 5 6

chain bonds :
2-9 6-8 7-8 7-14 8-11 11-12

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :
1-2 1-6 2-3 2-9 3-4 4-5 5-6 7-14 11-12

exact bonds :
6-8 7-8 8-11

G1:C,H,O,S,N,P

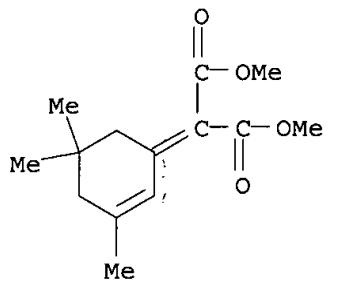
G2:C,H,O,N,p-C6H4,CO2H,CN

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS 14:CLASS

RN 124648-10-8 REGISTRY
 CN Propanedioic acid, (3,5,5-trimethyl-2-cyclohexen-1-ylidene)-, dimethyl ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C14 H20 O4
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier RID	RID Occurrence Count
EA	ES	SZ	RF	RID	
C6	C6	6	C6	46.150.2	1



A : COOR_e

COOR_f

R_c, R_f = Me

(D = CH₃, R_o, R_p = CH₃)

Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	580	pH 1	(1) ACD
Bioconc. Factor (BCF)	580	pH 4	(1) ACD
Bioconc. Factor (BCF)	580	pH 7	(1) ACD
Bioconc. Factor (BCF)	580	pH 8	(1) ACD
Bioconc. Factor (BCF)	580	pH 10	(1) ACD
Boiling Point (BP)	291.1 +/- 13.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	53.05 +/- 3.0 kJ/mol		(1) ACD
Flash Point (FP)	132.2 +/- 32.8 deg C		(1) ACD
H acceptors (HAC)	4		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3309	pH 1	(1) ACD
Koc (KOC)	3309	pH 4	(1) ACD
Koc (KOC)	3309	pH 7	(1) ACD
Koc (KOC)	3309	pH 8	(1) ACD
Koc (KOC)	3309	pH 10	(1) ACD
logD (LOGD)	3.94	pH 1	(1) ACD
logD (LOGD)	3.94	pH 4	(1) ACD
logD (LOGD)	3.94	pH 7	(1) ACD
logD (LOGD)	3.94	pH 8	(1) ACD
logD (LOGD)	3.94	pH 10	(1) ACD
logP (LOGP)	3.939 +/- 0.367		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD

Molecular Weight (MW)	252.31	(1) ACD
Vapor Pressure (VP)	0.00199311 Torr	25.0 deg C (1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

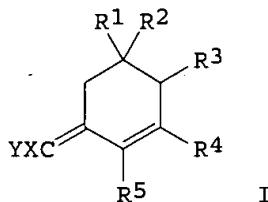
REFERENCE 1

AN 112:42246 CA
 TI Cyclohexenylidenes as sunscreen agents
 IN Cleary, Thomas P.; Gosciniak, Donald J.; Phalangas, Charalambos J.
 PA ICI Americas, Inc., USA
 SO U.S., 7 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 IC ICM A61K007-40
 ICS A61K007-42; A61K007-44; A61K009-10
 NCL 424059000
 CC 62-4 (Essential Oils and Cosmetics)
 Section cross-reference(s): 24

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4847073	A	19890711	US 1988-212824	19880629
	BR 8903225	A	19910102	BR 1989-3225	19880629
	EP 349139	A2	19900103	EP 1989-305854	19890609
	EP 349139	A3	19900530		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	ZA 8904488	A	19900725	ZA 1989-4488	19890613
	AU 8936362	A1	19900104	AU 1989-36362	19890614
	AU 616273	B2	19911024		
	FI 8903132	A	19891230	FI 1989-3132	19890627
	JP 02153988	A2	19900613	JP 1989-168256	19890629
PRAI	US 1988-212824		19880629		
	GB 1989-13345		19890609		

GI



AB Sunscreen compns. contain cyclohexenylidenes (I: X, Y = CN, CO₂R₆, CONHR₆, CONR₃2, PhCO₂R₆, PhCOR₆, PhNR₃2, only one X or Y may be substituted with H; R₁-R₅ = H, OH, CO₂R₆, alkyl, alkoxy, hydroxyalkyl; R₆ = H, alkyl, alkylaryl, arylalkyl) as UV filters. I provide selected absorption of actinic radiation in the UV-B as well as UV-A range. A mixt. contg. I (R₁-R₃ = H, R₄ = Me, R₅ = H, X = CN, Y = CO₂Me) (II) 8% and dimethylisosorbide 92% was applied to excised hairless mouse epidermis at 1 mg/cm² and the epidermis was exposed to UV radiation and the skin protection factor was measured to be 14.0 in the UV-B range and 1.73 in the UV-A range. A sunscreen lotion contained II 5.00, petrolatum 35.00, Brij-721 1.16, Brij-72 3.86, silicone oil 3.00, Uvinul M-40 3.00, water 48.08, Carbopol-934 0.40, NaOH (10% aq. soln.) 0.40, and Dowicil-200

0.10%.

ST sunscreen cyclohexenylidene cyanoacetate prepn

IT Polishing materials
(cyclohexenylidenes in, as sunscreen agents)

IT Hair preparations
Sunburn and Suntan
(sunscreens, cyclohexenylidenes in)

IT 109-73-9, Butylamine, biological studies
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of cyclohexenylidene cyanoacetic acid chloride)

IT 78-59-1, Isophorone
RL: BIOL (Biological study)
(condensation of, with Me cyanoacetate)

IT 62-53-3, Aniline, biological studies 67-63-0, Isopropanol, biological studies 126-30-7, 2,2-Dimethyl-1,3-propanediol
RL: BIOL (Biological study)
(condensation of, with cyclohexenylidene cyanoacetate)

IT 105-34-0, Methyl cyanoacetate 108-59-8, Dimethyl malonate
RL: BIOL (Biological study)
(condensation of, with isophorone)

IT 124648-13-1P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(prep. and amidation of, with butylamine)

IT 56058-30-1P 124648-14-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prep. and condensation of, with Et cyanoacetate)

IT 80699-65-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prep. and reaction of, with crotonaldehyde)

IT 30525-89-4, Paraformaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et acetoacetate)

IT 4170-30-3, Crotonaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with isophorone silyl enol ether)

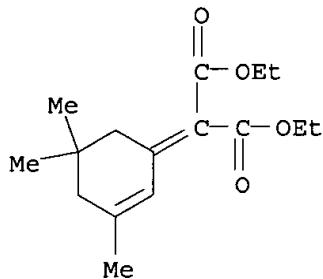
IT 141-97-9, Ethyl acetoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with paraformaldehyde)

IT 20159-49-3 23051-44-7 52903-68-1 52903-69-2 55952-69-7
88973-42-6 107100-75-4 124647-97-8 124647-98-9 124647-99-0
124648-00-6 124648-01-7 124648-02-8 124648-03-9 124648-04-0
124648-05-1 124648-06-2 124648-07-3 124648-08-4 124648-09-5
124648-10-8 124648-11-9 124648-12-0
RL: BIOL (Biological study)
(sunscreen agent)

RN 41589-44-0 REGISTRY
 CN Propanedioic acid, (3,5,5-trimethyl-2-cyclohexen-1-ylidene)-, diethyl ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C16 H24 O4
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.2	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	3725	pH 1	(1) ACD
Bioconc. Factor (BCF)	3725	pH 4	(1) ACD
Bioconc. Factor (BCF)	3725	pH 7	(1) ACD
Bioconc. Factor (BCF)	3725	pH 8	(1) ACD
Bioconc. Factor (BCF)	3725	pH 10	(1) ACD
Boiling Point (BP)	325.0 +/- 15.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	56.71 +/- 3.0 kJ/mol		(1) ACD
Flash Point (FP)	148.6 +/- 33.8 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	4		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	12526	pH 1	(1) ACD
Koc (KOC)	12526	pH 4	(1) ACD
Koc (KOC)	12526	pH 7	(1) ACD
Koc (KOC)	12526	pH 8	(1) ACD
Koc (KOC)	12526	pH 10	(1) ACD
logD (LOGD)	5.00	pH 1	(1) ACD
logD (LOGD)	5.00	pH 4	(1) ACD
logD (LOGD)	5.00	pH 7	(1) ACD
logD (LOGD)	5.00	pH 8	(1) ACD
logD (LOGD)	5.00	pH 10	(1) ACD
logP (LOGP)	5.002 +/- 0.367		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	280.36		(1) ACD
Vapor Pressure (VP)	0.000236805 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

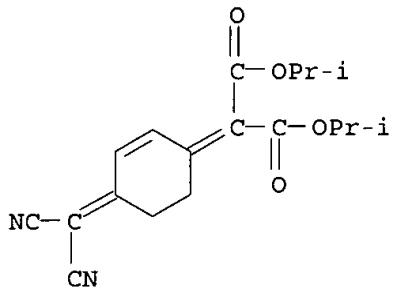
REFERENCE 1

AN 78:158864 CA
 TI Knoevenagel condensations with titanium tetrachloride-base. III.
 Reaction of ketones and .alpha.-halo ketones with malonate
 AU Lehnert, W.
 CS Univ.-Kinderklin., Freiburg, Fed. Rep. Ger.
 SO Tetrahedron (1973), 29(4), 635-8
 CODEN: TETRAB; ISSN: 0040-4020
 DT Journal
 LA German
 CC 23-16 (Aliphatic Compounds)
 Section cross-reference(s): 24, 25, 26
 AB Condensation of H₂C(CO₂Et)₂ with aliph., arom., and cyclic ketones, RR₁CO,
 in the presence of TiCl₄-pyridine gave 42-96% RR₁C:C(CO₂Et)₂. .alpha.-Mono-
 , .alpha., .alpha.-di-, and .alpha., .alpha., .alpha.-trihalo ketones reacted
 similarly.
 ST Knoevenagel malonate ketone; halo ketone malonate Knoevenagel; titanium
 chloride Knoevenagel
 IT Ketones, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Knoevenagel condensation of, with diethyl malonate)
 IT Knoevenagel reaction
 (of ketones with diethyl malonate in presence of titanium
 tetrachloride-pyridine)
 IT 7550-45-0, uses and miscellaneous
 RL: USES (Uses)
 (Knoevenagel condensation of ketones with diethyl malonate in presence
 of pyridine and)
 IT 110-86-1, uses and miscellaneous
 RL: USES (Uses)
 (Knoevenagel condensation of ketones with diethyl malonate in presence
 of titanium tetrachloride and)
 IT 108-59-8
 RL: RCT-(Reactant); RACT (Reactant or reagent)
 (Knoevenagel condensation of, with bicycloheptanone)
 IT 67-64-1, reactions 78-59-1 78-93-3, reactions 78-95-5 108-94-1,
 reactions 119-61-9, reactions 120-92-3 123-19-3 134-81-6
 421-50-1 486-25-9 497-38-1 532-27-4 534-07-6 1191-95-3
 2648-61-5 4091-39-8 6317-49-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Knoevenagel condensation of, with diethyl malonate)
 IT 105-53-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Knoevenagel condensation with ketones of, in presence of titanium
 tetrachloride-pyridine)
 IT 6802-75-1P 24824-36-0P 41589-39-3P 41589-40-6P 41589-41-7P
 41589-42-8P 41589-43-9P 41589-44-0P 41589-45-1P 41589-46-2P
 41589-48-4P 41589-49-5P 41589-50-8P 41589-51-9P 41589-52-0P
 41589-53-1P 41589-54-2P 41649-47-2P 41649-48-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep. of)

RN 199384-77-5 REGISTRY
 CN Propanedioic acid, [4-(dicyanomethylene)-2-cyclohexen-1-ylidene] - ,
 bis(1-methylethyl) ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C18 H20 N2 O4
 SR CA
 LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier RID	RID Occurrence Count
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.2	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	98.8	pH 1	(1) ACD
Bioconc. Factor (BCF)	98.8	pH 4	(1) ACD
Bioconc. Factor (BCF)	98.8	pH 7	(1) ACD
Bioconc. Factor (BCF)	98.8	pH 8	(1) ACD
Bioconc. Factor (BCF)	98.8	pH 10	(1) ACD
Boiling Point (BP)	421.9+/-45.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	67.60+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	184.4+/-34.1 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	932	pH 1	(1) ACD
Koc (KOC)	932	pH 4	(1) ACD
Koc (KOC)	932	pH 7	(1) ACD
Koc (KOC)	932	pH 8	(1) ACD
Koc (KOC)	932	pH 10	(1) ACD
logD (LOGD)	2.93	pH 1	(1) ACD
logD (LOGD)	2.93	pH 4	(1) ACD
logD (LOGD)	2.93	pH 7	(1) ACD
logD (LOGD)	2.93	pH 8	(1) ACD
logD (LOGD)	2.93	pH 10	(1) ACD
logP (LOGP)	2.928+/-0.437		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	328.36		(1) ACD
Vapor Pressure (VP)	2.51E-07 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 128:23197 CA
 TI Synthesis and polymerization of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes
 AU Itoh, Takahito; Okuno, Hiroyuki; Hishida, Takeshi; Inokuchi, Akira; Kamei, Nobuaki; Sato, Tamotsu; Kubo, Masataka; Iwatsuki, Shouji
 CS Dep. Chem. Mater., Fac. Eng., Mie Univ., Mie, 514, Japan
 SO Tetrahedron (1997), 53(45), 15247-15261
 CODEN: TETRAB; ISSN: 0040-4020
 PB Elsevier
 DT Journal
 LA English
 CC 35-4 (Chemistry of Synthetic High Polymers)
 AB Attempts were made to prep. novel 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes [ethoxy(5a), isopropoxy(5b), and tert-butoxy(5c)], 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes [ethoxy(6a), isopropoxy(6b), and tert-butoxy(6c)], and 1-(2,2-dimethyl-1,3-dioxane-4,6-dione-5-ylidene)-4-(dicyanomethylene)-2,5-cyclohexadiene(6d). 5c and 6d were obtained as yellow and orange needles, resp., but 5a, 5b and 6a-c could not be isolated as crystals. Homopolymns. of 5c and 6d and their copolymns. with styrene were studied.
 ST alkoxy carbonyl tricyanoquinodimethane bis alkoxy carbonyl dicyanoquinodimethane prepn polymn
 IT Polymerization
 Polymerization catalysts
 (ionic; synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)
 IT Polymerization
 Polymerization catalysts
 (radical; synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)
 IT Carbo polymers
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthesis and polymn. of 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)
 IT Solvent effect
 (synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)
 IT 199384-59-3P 199384-60-6P 199384-61-7P 199384-62-8P 199384-63-9P
 199384-64-0P 199384-65-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (monomer; synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)
 IT 78-67-1, AIBN 109-63-7, Boron trifluoride etherate 109-72-8, Butyl lithium, uses 121-44-8, uses 616-45-5, Pyrrolidone
 RL: CAT (Catalyst use); USES (Uses)
 (polymn. catalyst; synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-

tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)

IT 199384-69-5P 199384-70-8P 199384-71-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)

IT 105-53-3, Diethyl malonate 109-77-3, Malonodinitrile 541-16-2,
Di(tert-butyl) malonate 2033-24-1, Isopropylidene malonate 13195-64-7,
Diisopropyl malonate 83928-81-8 83928-82-9 145984-88-9 156879-16-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)

IT 199384-66-2P 199384-67-3P 199384-68-4P 199384-72-0P 199384-73-1P
199384-74-2P 199384-75-3P 199384-76-4P 199384-77-5P 199384-78-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)

IT 199384-79-7P 199384-80-0P 199384-81-1P 199384-82-2P 199384-83-3P
199384-84-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)

AN 2000:409546 CAPLUS
DN 133:230235
TI Influence of the chromophore ionization potential on speed and magnitude of photorefractive effects in poly(N-vinylcarbazole) based polymer composites
AU Van Steenwinckel, David; Hendrickx, Eric; Persoons, Andre; Van den Broeck, Kurt; Samyn, Celest
CS Center for Research on Molecular Electronics and Photonics, Laboratory for Chemical and Biological Dynamics, University of Leuven, Louvain, B-3001, Belg.
SO J. Chem. Phys. (2000), 112(24), 11030-11037
CODEN: JCPSA6; ISSN: 0021-9606
PB American Institute of Physics
DT Journal
LA English
CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 73
AB The authors report on the synthesis of three highly polar chromophores and their use as **dopants** in poly(N-vinylcarbazole) based photorefractive polymer composites sensitized with (2,4,7-trinitro-9-fluorenylidene)malononitrile. Small alterations in the amino donor group substituents were used to tune the dye's ionization potential (IP) by 0.2 eV. At 780 nm, 5 .degree.C above the glass transition temp. (Tg), and with an applied field of 59 V/.mu.m, the authors obsd. complete internal diffraction and a gain coeff. of 167 cm⁻¹. In this temp. range, diffraction efficiency, gain coeff., and photorefractive phase shift were found to correlate with the chromophore IP. At 20 .degree.C Tg, the contribution from birefringence to the index modulation was insignificant, and the speed of the photorefractive effect correlated well with the chromophore IP. Anal. of the results suggests that the space-charge field was influenced by the chromophore IP.
ST photorefractive effect polyvinylcarbazole based polymer composite; chromophore ionization potential photorefractive effect polyvinylcarbazole based polymer composite
IT Ionization potential
Photorefractive effect
Photorefractive gratings (chromophore **dopant** ionization potential effect on photorefractive effects in poly(vinylcarbazole) based polymer composites)
IT 149227-09-8 190715-16-3 190715-17-4
RL: MOA (Modifier or additive use); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process); USES (Uses) (chromophore **dopant** ionization potential effect on photorefractive effects in poly(vinylcarbazole) based polymer composites)
IT 25067-59-8, Poly(N-vinylcarbazole)
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process) (chromophore **dopant** ionization potential effect on

photorefractive effects in poly(vinylcarbazole) based polymer composites)

IT 86-28-2, N-Ethylcarbazole
 RL: NUU (Nonbiological use, unclassified); USES (Uses)
 (plasticizer; chromophore **dopant** ionization potential effect
 on photorefractive effects in poly(vinylcarbazole) based polymer composites)

IT 1201-91-8, 4-[N-(2-Hydroxyethyl)-N-methylamino]benzaldehyde 4181-05-9,
 p-N,N-Diphenylaminobenzaldehyde 42906-19-4, 4-N,N-Di-(p-tolyl)aminobenzaldehyde
 RL: RCT (Reactant)
 (reaction with (trimethylhexeneylidene)propanedinitrile)

IT 23051-44-7
 RL: RCT (Reactant)
 (reaction with aminobenzaldehydes)

IT 1172-02-7, 2,4,7-Trinitro-9-fluorenylidene)malononitrile
 RL: MOA (Modifier or additive use); USES (Uses)
 (sensitizer; chromophore **dopant** ionization potential effect
 on photorefractive effects in poly(vinylcarbazole) based polymer composites)

RE.CNT 29

RE

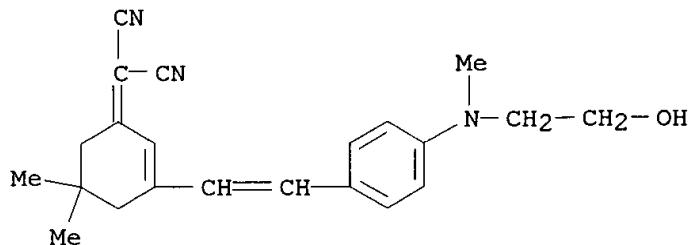
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IT 149227-09-8 190715-16-3 190715-17-4
 RL: MOA (Modifier or additive use); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process); USES (Uses)
 (chromophore **dopant** ionization potential effect on

photorefractive effects in poly(vinylcarbazole) based polymer
composites)

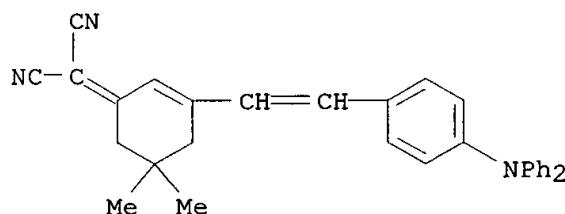
RN 149227-09-8 CAPLUS

CN Propanedinitrile, [3-[2-[4-[(2-hydroxyethyl)methylamino]phenyl]ethenyl]-
5,5-dimethyl-2-cyclohexen-1-ylidene]- (9CI) (CA INDEX NAME)



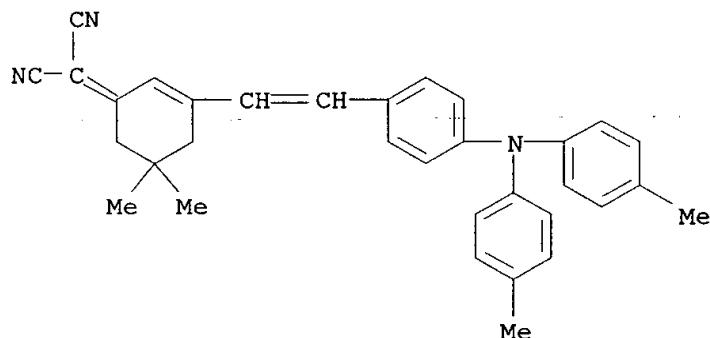
RN 190715-16-3 CAPLUS

CN Propanedinitrile, [3-[2-[4-(diphenylamino)phenyl]ethenyl]-5,5-dimethyl-2-
cyclohexen-1-ylidene]- (9CI) (CA INDEX NAME)



RN 190715-17-4 CAPLUS

CN Propanedinitrile, [3-[2-[4-[bis(4-methylphenyl)amino]phenyl]ethenyl]-5,5-
dimethyl-2-cyclohexen-1-ylidene]- (9CI) (CA INDEX NAME)



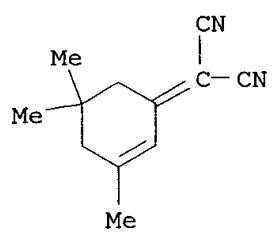
IT 23051-44-7

RL: RCT (Reactant)

(reaction with aminobenzaldehydes)

RN 23051-44-7 CAPLUS

CN Propanedinitrile, (3,5,5-trimethyl-2-cyclohexen-1-ylidene)- (9CI) (CA
INDEX NAME)



AN 1999:601885 CAPLUS
DN 131:345185
TI Colorless high dielectric compounds for low voltage liquid crystal application
AU Wu, Shin-Tson; Schwartz, Robert N.; Zhang, Qing T.; Marder, Seth; Hsu, Chain-Shu
CS HRL Laboratories, Malibu, CA, 90265, USA
SO Mater. Res. Soc. Symp. Proc. (1999), 559(Liquid Crystal Materials and Devices), 235-242
CODEN: MRSPDH; ISSN: 0272-9172
PB Materials Research Society
DT Journal
LA English
CC 76-9 (Electric Phenomena)
Section cross-reference(s): 74, 75
AB Several colorless compds. with dielec. anisotropy in the 10-50 range were studied. The absorption spectra, phase transition temp., birefringence, dielec. anisotropy and viscoelastic coeff. of these compds. were measured.
ST dielec compd liq crystal
IT Liquid crystal displays
 (active matrix; colorless high dielec. compds. for low voltage liq. crystal application)
IT Absorption spectra
Birefringence
Dielectric anisotropy
Dielectric constant
Electric insulators
 Liquid crystals
Viscosity
 (colorless high dielec. compds. for low voltage liq. crystal application)
IT Polyenes
RL: PRP (Properties)
 (cyano-; colorless high dielec. compds. for low voltage liq. crystal application)
IT 23051-44-7 27104-69-4 30481-43-7 68162-22-1
74240-64-5 74701-06-7 86776-50-3 117530-21-9 154195-65-0
190602-28-9 190602-29-0 190602-31-4 220036-97-5 249934-22-3
249934-23-4 249934-24-5
RL: PRP (Properties)
 (colorless high dielec. compds. for low voltage liq. crystal application)
RE.CNT 18
RE
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IT 23051-44-7 30481-43-7 249934-22-3

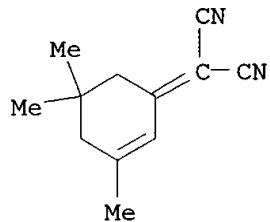
249934-23-4

RL: PRP (Properties)

(colorless high dielec. compds. for low voltage liq.
 crystal application)

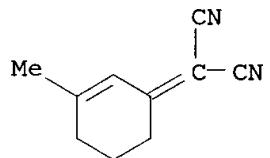
RN 23051-44-7 CAPLUS

CN Propanedinitrile, (3,5,5-trimethyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX NAME)



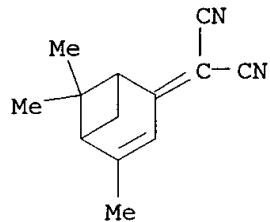
RN 30481-43-7 CAPLUS

CN Propanedinitrile, (3-methyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX NAME)



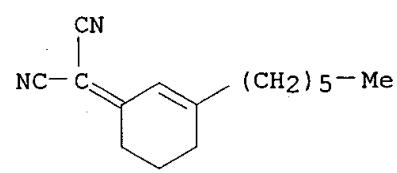
RN 249934-22-3 CAPLUS

CN Propanedinitrile, (4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-ylidene)- (9CI) (CA INDEX NAME)



RN 249934-23-4 CAPLUS

CN Propanedinitrile, (3-hexyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX NAME)



AN 2000:725601 CAPLUS
DN 133:303666
TI **Dopants for liquid crystal devices**
IN Wu, Shin-tson; Marder, Seth; Zhang, Qing T.
PA Hrl Laboratories, Llc, USA; California Institute of Technology
SO PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07C255-31
ICS C09K019-58
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 24, 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000059872	A1	20001012	WO 2000-US8488	20000329
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			

PRAI US 1999-285937 A1 19990402

AB High-dielec. colorless or virtually colorless **dopants** for low-voltage and tunable clearing temp. **liq. crystal** devices. These **dopant** compds. help reduce the operation voltage for both polar and non-polar **liq. crystal** (LC) mixts. Methods for making and using these **dopant** compds. are also disclosed.

ST **liq crystal display dopant**

IT **Dopants**

Liquid crystal displays
(dopants for liq. crystal devices)

IT 23051-44-7P 30481-43-7P 249934-23-4P

300859-99-8P

RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(dopants for liq. crystal devices)

IT 78-59-1 109-77-3, Malononitrile 1193-18-6 1196-01-6 3761-92-0,
Hexylmagnesium bromide 5323-87-5 66262-12-2

RL: RCT (Reactant)

(dopants for liq. crystal devices)

RE.CNT 8

RE

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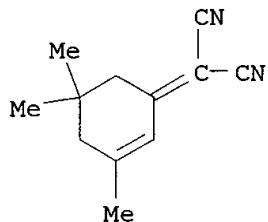
IT 23051-44-7P 30481-43-7P 249934-23-4P

300859-99-8P

RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)
(dopants for liq. crystal devices)

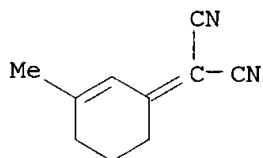
RN 23051-44-7 CAPLUS

CN Propanedinitrile, (3,5,5-trimethyl-2-cyclohexen-1-ylidene)- (9CI) (CA
INDEX NAME)



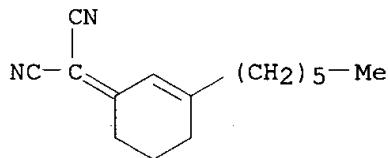
RN 30481-43-7 CAPLUS

CN Propanedinitrile, (3-methyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX
NAME)



RN 249934-23-4 CAPLUS

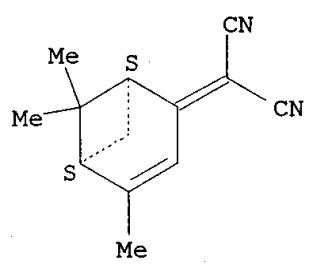
CN Propanedinitrile, (3-hexyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX
NAME)



RN 300859-99-8 CAPLUS

CN Propanedinitrile, [(1S,5S)-4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-
ylidene]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



AN 1992:407540 CAPLUS
DN 117:7540
ED Entered STN: 11 Jul 1992
TI Reactions of trifluoromethyl ketones. VIII. Investigation of steric effect of a trifluoromethyl group through ene reaction of trifluoromethyl ketones
AU Nagai, Takabumi; Nishioka, Goro; Koyama, Mayumi; Ando, Akira; Miki, Takuichi; Kumadaki, Itsunaro
CS Fac. Pharm. Sci., Setsunan Univ., Hirakata, 573-01, Japan
SO Chemical & Pharmaceutical Bulletin (1992), 40(3), 593-8
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 22
OS CASREACT 117:7540
AB In the ene reaction of trifluoromethyl ketones, a trifluoromethyl group has been obsd. to behave as a larger substituent than commonly believed in the biomedicinal field. To est. the steric effect of a trifluoromethyl group, several trifluoromethyl ketones RCOCF₃ (R = H, Me, Bu, Ph, Me₂CHCH₂, cyclohexyl, EtMeCH, CF₃, thexyl) were prepnd. and their ene reaction with cyclohexene, a 1,2-disubstituted ene having the least steric requirement, examd. In this reaction, a trifluoromethyl group was found to behave as if it were a much larger substituent than a Ph or iso-Bu group and as large as a sec-Bu group.
ST steric effect trifluoromethyl group ene reaction; ketone trifluoromethyl ene reaction; stereochem ene reaction trifluoromethyl ketone; regiochem ene reaction trifluoromethyl ketone
IT Steric effect
(of trifluoromethyl group on ene reaction of trifluoromethyl ketones)
IT Trifluoromethyl group
(steric effect of, on ene reactions of trifluoromethyl ketones)
IT Addition reaction
(ene, of trifluoromethyl ketones, steric effect of trifluoromethyl group on)
IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(trifluoromethyl, ene reaction of, steric effect of trifluoromethyl group on)
IT 76-05-1, Trifluoroacetic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of)
IT 108-85-0, Cyclohexyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with iso-Bu trifluoromethyl ketone)
IT 78-77-3, Isobutyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with trifluoroacetic acid)
IT 1521-51-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with trifluoroacetophenone)
IT 75-90-1, Trifluoroacetaldehyde 360-34-9 421-50-1 434-45-7,
.alpha.,.alpha.,.alpha.-Trifluoroacetophenone 684-16-2,
Hexafluoroacetone
RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, steric effect of the trifluoromethyl group in)
IT 433-27-2, Trifluoroacetaldehyde ethyl hemiacetal
RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, with dimethylbutenes)
IT 563-79-1, 2,3-Dimethyl-2-butene
RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, with trifluoroacetaldehyde)
IT 110-83-8, Cyclohexene, reactions 13389-42-9
RL: RCT (Reactant); RACT (Reactant or reagent)

(ene reaction of, with trifluoromethyl ketones)

IT 116356-54-8P 122129-36-6P 122129-38-8P 141779-27-3P 141779-28-4P
 141779-29-5P 141779-30-8P 141779-31-9P 141779-32-0P
 141779-33-1P 141779-34-2P 141779-35-3P 141779-36-4P
141779-37-5P 141779-38-6P 141779-39-7P
 141779-42-2P 141779-43-3P 141779-44-4P 141846-75-5P 141846-76-6P
 141846-77-7P 141899-03-8P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prep. and spectra of)

IT 114420-54-1P 122129-28-6P 122129-29-7P 122129-30-0P 122129-31-1P
 125458-29-9P 134166-51-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep. of)

IT 134166-52-2P 134166-53-3P 134166-54-4P 134166-55-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep., spectra and dehydration of)

IT 6302-04-1P, Cyclohexyl trifluoromethyl ketone 75703-02-5P, Isobutyl trifluoromethyl ketone 134166-49-7P, sec-Butyl trifluoromethyl ketone 134166-50-0P, Thexyl trifluoromethyl ketone
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep., spectra and ene reaction of, steric effect of the trifluoromethyl group in)

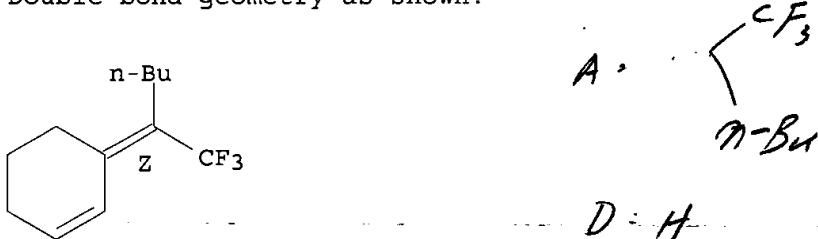
IT 141779-40-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep., spectra and hydrogenation of)

IT 141779-41-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep., spectra and oxidn. of)

IT 141779-32-0P 141779-34-2P 141779-35-3P
 141779-37-5P 141779-38-6P 141779-39-7P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prep. and spectra of)

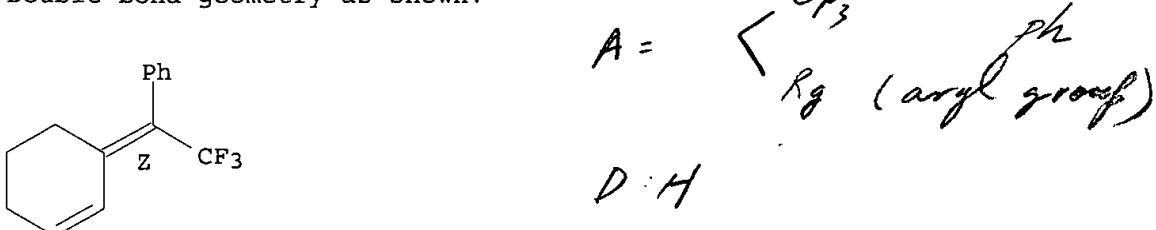
RN 141779-32-0 CAPPLUS
 CN Cyclohexene, 3-[1-(trifluoromethyl)pentylidene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 141779-34-2 CAPPLUS
 CN Benzene, [1-(2-cyclohexen-1-ylidene)-2,2,2-trifluoroethyl]-, (Z)- (9CI)
 (CA INDEX NAME)

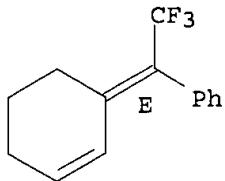
Double bond geometry as shown.



RN 141779-35-3 CAPPLUS
 CN Benzene, [1-(2-cyclohexen-1-ylidene)-2,2,2-trifluoroethyl]-, (E)- (9CI)

(CA INDEX NAME)

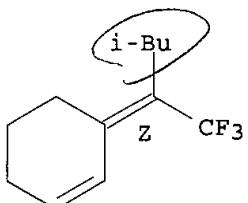
Double bond geometry as shown.



RN 141779-37-5 CAPLUS

CN Cyclohexene, 3-[3-methyl-1-(trifluoromethyl)butylidene]-, (Z)- (9CI) (CA
INDEX NAME)

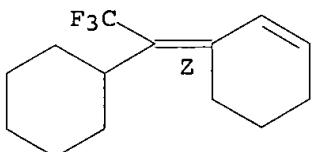
Double bond geometry as shown.



RN 141779-38-6 CAPLUS

CN Cyclohexene, 3-(1-cyclohexyl-2,2,2-trifluoroethylidene)-, (Z)- (9CI) (CA
INDEX NAME)

Double bond geometry as shown.



RN 141779-39-7 CAPLUS

CN Cyclohexene, 3-(1-cyclohexyl-2,2,2-trifluoroethylidene)-, (E)- (9CI) (CA
INDEX NAME)

Double bond geometry as shown.

